Support information

Conversion of biomass-derived monosaccharides to 2-methylfuran in supercritical acetone

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Table S1 The conversion of fructose.

Entry	T (℃)	Time (h)	Conversion (%)
1	260	2	100
2	260	4	100
3	260	6	100
4	260	8	100
5	260	10	100

Reaction conditions: 100 mg fructose, 50 mL acetone, 2 MPa N_2, 260 ℃, 2h.

Table S2 The conversion of glucose.

Entry	T (℃)	Time (h)	Conversion (%)
1	260	0.5	100
2	260	1	100
3	260	1.5	100
4	260	2	100
5	260	4	100
6	260	6	100

Reaction conditions: 100 mg glucose, 50 mL acetone, 2 MPa N_2, 260 ℃, 2h.

Table S3 The conversion of xylose.

Entry	T (℃)	Time (h)	Conversion (%)
1	260	2	100
2	260	4	100
3	260	6	100
4	260	8	100
5	260	10	100
6	260	12	100
7	260	14	100

Reaction conditions: 100 mg xylose, 50 mL acetone, 2 MPa N_2, 260 ℃, 2h.

Table S4 The conversion of xylose at different dosages of water.

Entry	H_2O （mL）	Xylose (mg)	T (℃）	Time (h)	Conversion (%)
1	1	100	260	2	100
2	3	100	260	2	100
3	5	100	260	2	100
4	7	100	260	2	100
5	9	100	260	2	100
6	11	100	260	2	100
7	13	100	260	2	100
8	15	100	260	2	100
9	17	100	260	2	100

Reaction conditions: 100 mg xylose, water and acetone 50 mL, 2 MPa N_2, 260 ℃, 2h.

Table S5 The conversion of xylose at different reaction temperature.

Entry	H_2O （mL）	Xylose (mg)	T (℃）	Time (h)	Conversion (%)
1	11	100	140	2	0
2	11	100	180	2	50
3	11	100	220	2	63
4	11	100	260	2	100
5	11	100	280	2	100

Reaction conditions: 100 mg xylose, water and acetone 50 mL, 2 MPa N_2, 260 ℃, 2h.

Table S6 The conversion of xylose at different reaction time.

Entry	H_2O （mL）	Xylose (mg)	T (℃）	Time (h)	Conversion (%)
1	11	100	260	0.5	100
2	11	100	260	1	100
3	11	100	260	1.5	100
4	11	100	260	2	100
5	11	100	260	2.5	100

Reaction conditions: 100 mg xylose, water and acetone 50 mL, 2 MPa N_2, 260 ℃, 2h.

Table S7 The conversion of xylose at different dosages of xylose.

Entry	H_2O （mL）	Xylose (mg)	T (℃）	Time (h)	Conversion (%)
1	11	50	260	2	100
2	11	100	260	2	100
3	11	150	260	2	100
4	11	200	260	2	100
5	11	250	260	2	100
6	11	300	260	2	100
7	11	350	260	2	100

Reaction conditions: 100 mg xylose, water and acetone 50 mL, 2 MPa N_2, 260 ℃, 2h.

Table S8 TOF analysis for reaction pathways.

Entry	Pathway	TDI	TDTS	ΔΔG (kcal/mol)	ΔGr (kcal/mol)	TOF (s^{-1})
1	2-MF	B-IM3	B-TS3	24.7	-24	3.82E+02
2	MLK	B-IM11	A-TS21	27.7	-9.2	2.87E+01
3	DFR	B-IM13	B-TS17	31.3	-34.7	1.05E+00

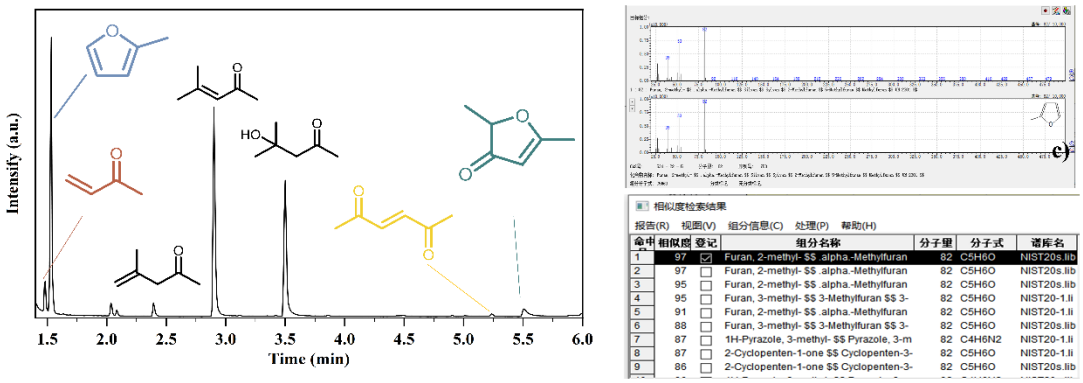

Fig. S1. GC-MS of the products from xylose in supercritical acetone. Reaction conditions: 100 mg xylose, 50 mL acetone, 2 MPa N_2, 260 ℃, 2h.

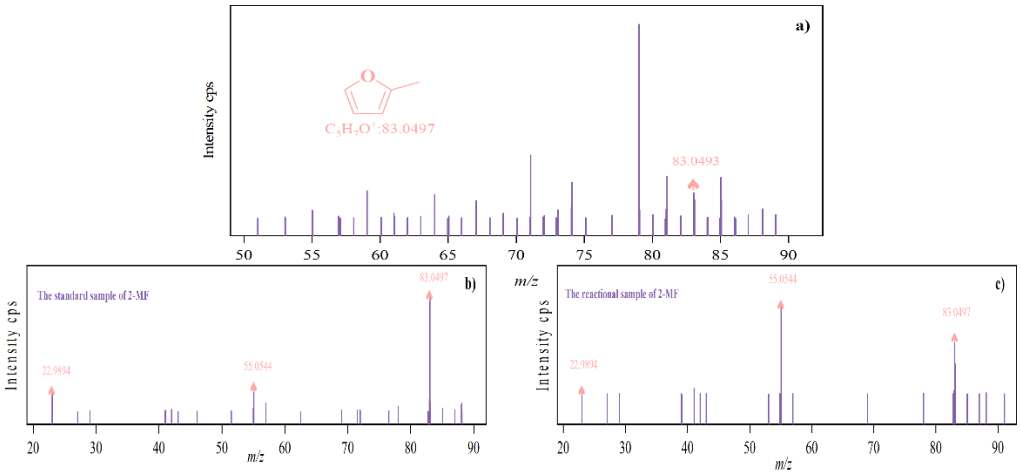

Fig. S2. ESI-MS for 2-MF from xylose conversion (a), ESI-MSMS for 2-MF from standard sample (b) and 2-MF from xylose conversion (c). Reaction conditions: 100 mg xylose, 50 mL acetone, 2 MPa N_2, 260 ℃, 2h.

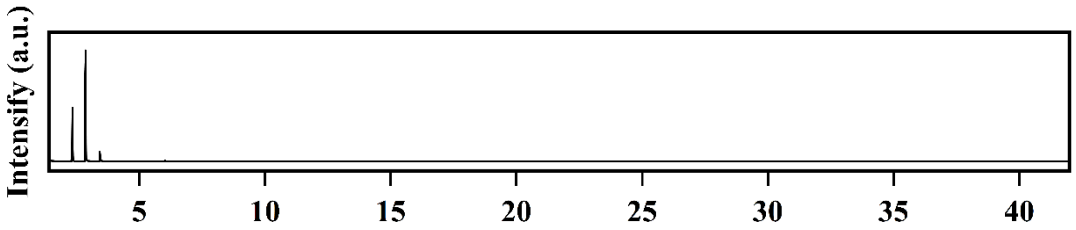

Fig. S3 GC-MS of the blank experiment of solvent. Reaction conditions: 50 mL acetone, 2 MPa N_2, 260 ℃, 2 h.

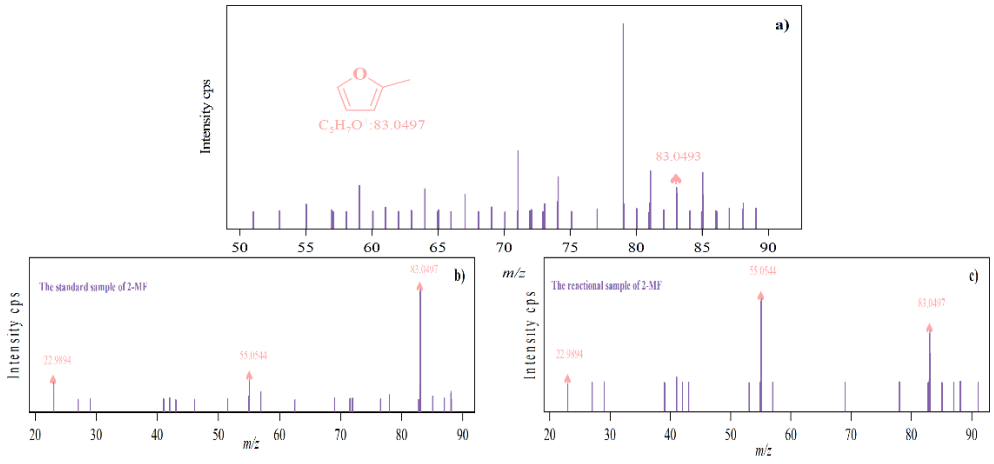

Fig. S4. ^{13}C NMR spectrum of 2-MF in DMSO-d6 (800 MHz). Reaction conditions: 100 mg xylose, 50 mL acetone, 2 MPa N_2, 260 ℃, 2h.

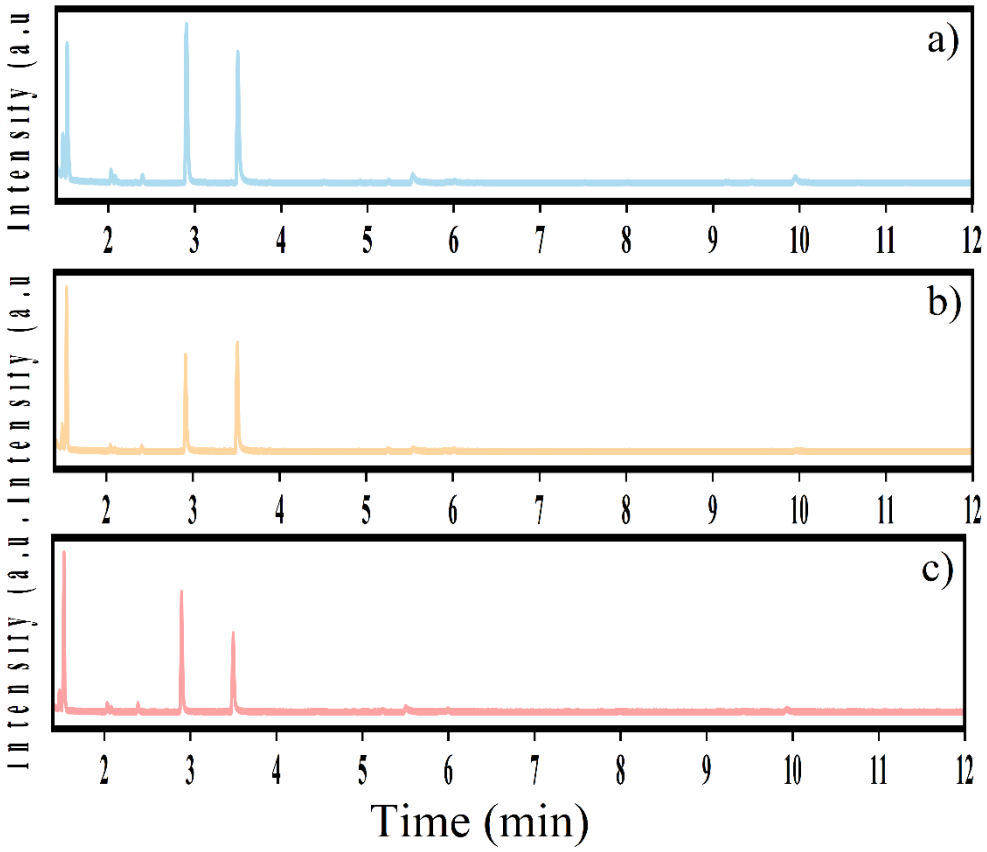

Fig. S5. GC-MS of the products from different monosaccharides in supercritical acetone. a)

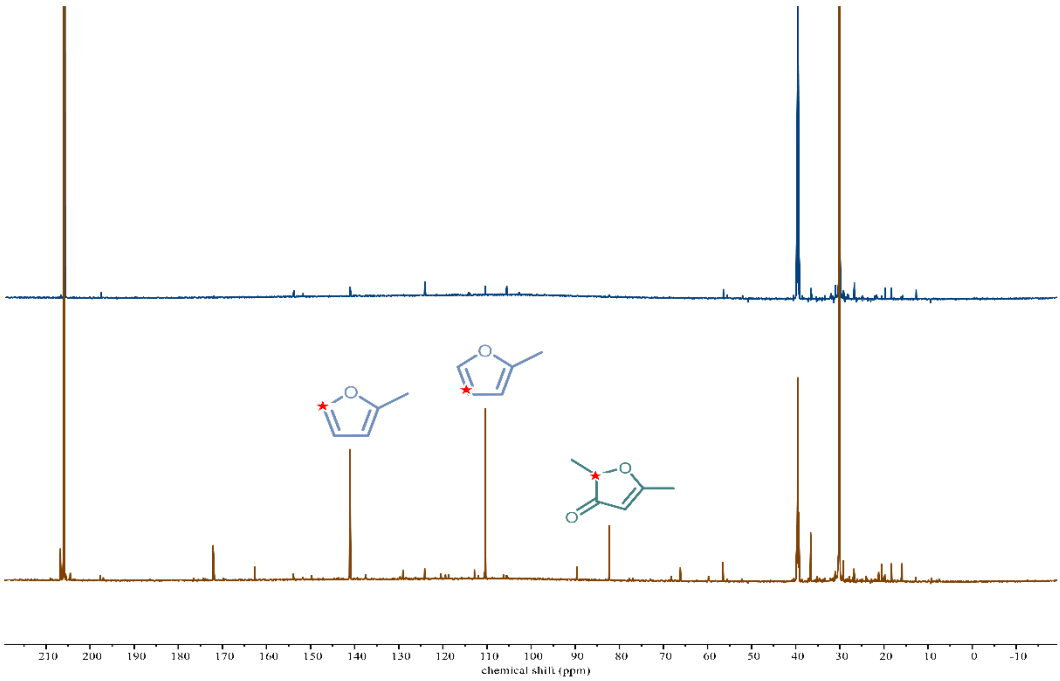

Fig. S6 ^{13}C NMR spectra of liquid products obtained from xylose (a: xylose, b: [4-^{13}C]-D-xylose). Reaction conditions: 90 mg xylose, 5.5 mL water and 19.5 mL acetone, 2 MPa N_2, 260 ℃, 2 h.

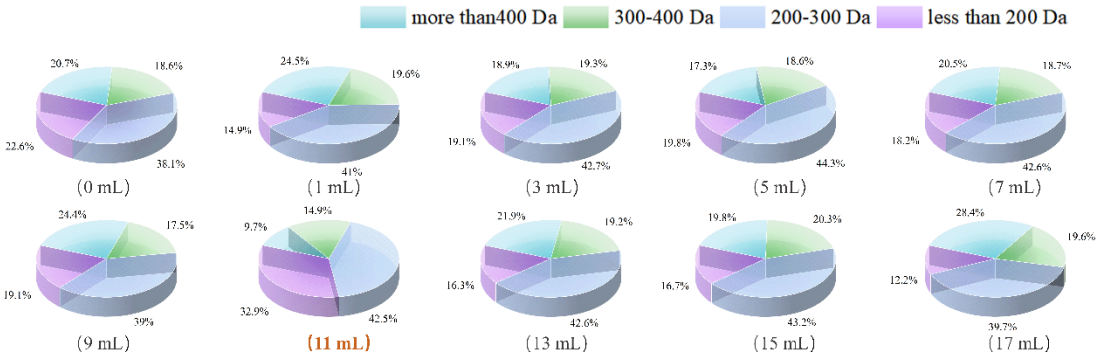

Fig. S7. Molecular weight distribution of xylose reaction solution at different dosages of water. Reaction conditions: 100 mg xylose, water and acetone 50 mL, 2 MPa N_2, 260 ℃, 2h.

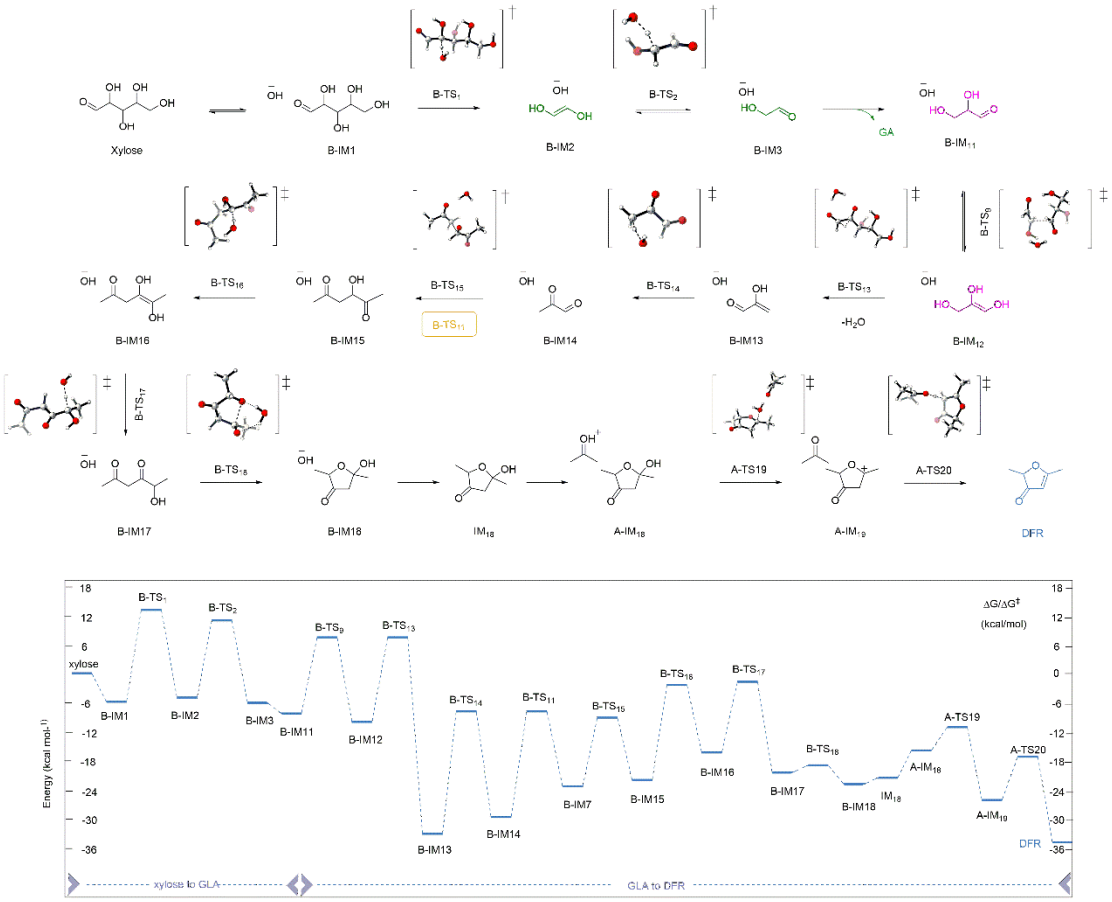

Fig. S8. The reaction mechanism of DFR. a) The schematic of the conversion of xylose to DFR; b) The energy diagram for DFR from xylose.

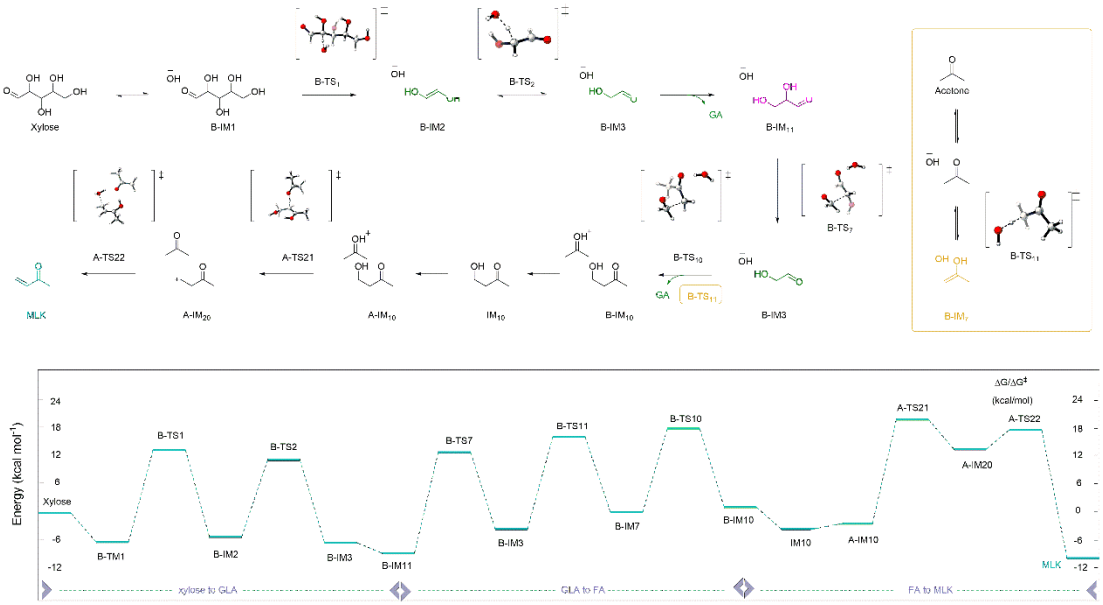

Fig. S9. The reaction mechanism of MLK. a) The schematic of the conversion of xylose to DFR; b) The energy diagram for MLK from xylose.